MULTI SCALE NUMERICAL SIMULATION OF COOPERATIVE CVD PROCESSES

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Reacting multiphase flows have attracted considerable attention due to their many industrial applications such as CVD-reactor, fluidized bed, combustion etc. In order to predict flow properties necessary for design purposes, there exits nowadays a hierarchy of models based on Euler-Lagrangian and pure Eulerian approach that are applied for two-phase flows. The models extend from the homogeneous ones valid for strongly coupled two-phase flows to two-liquid models valid for weakly coupled two-phase flows. We consider equations for isolated solid particle in a reacting carrier gas flow taking into account the detailed chemical kinetics at the particle surface as well as in a volume close to the particle (so called micro consideration, i.e. the mesoscale). The micro equations are accomplished with the balance equations for mass, momentum, and energy, averaged in a certain sense and expressed for each phase using only the Eulerian approach. The particle fractions are considered to take into account the mass and particle size variation. Two-phase reacting flows have been investigated in the past ten years. Chemical condensation processes (CCP) are connected with mutual influence of chemical reactions, heat-mass-transfer, and phase transition from gas to solid under non-stationary conditions. The kinetics of phase transition is accompanied by the super-saturation degree in the gas phase and strongly influences on the particle dispersion. In the intermediate stage of the phase transition the particle growth depends on appearance of new particle of a supercritical size. The super-saturation degree depends in its turn on the particle number density as well as on heat-mass transfer rate in the flow. Computation of cooperative CVD processes at a particle surface is performed. The relationship between macroscopic parameters in a reacting mixture and detailed kinetics of microscopic processes is considered. The basic set of the equations is the Navier-Stokes system supplemented by the terms resulting from microscopic analysis and averaging procedure along with relaxation equations for the chemical species. The governing equations represent the mass conservation for gas species, condensed particles and its fractions as well as the momentum, and energy conservation in a reacting flow. The new technique is developed in order to provide the stable algorithm for numerical simulation of a reacting two-phase flow in a tube. The approach uses the second order approximations on a nonuniform grid as well as the compact fifth-order advection term and fourth-order diffusion term approximations. As a result the processes whose scales differ from each other by orders of magnitude are examined. Using the composition of reagents and temperature condition, it is possible to control the structure of Al2O3 and its rate of production. The physico-chemical mathematical model of such processes including the spontaneous nucleation and particle growth are in progress. Based on the model kinetics scheme, the fields of temperature, mass fractions, and particle radius are presented for the various values of similarity parameters of the problem. The highly accurate method enables to control scales interaction and justifies various flow structures.

References

[1]A. Markov and A. Sadiki, "The Splitting Technique in Numerical Simulation of Two-phase Reacting Flows in a Tube," *Proc. of the Fifth World Congress on Computational Mechanics. Vienna,* , 2002.